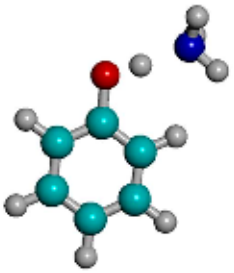

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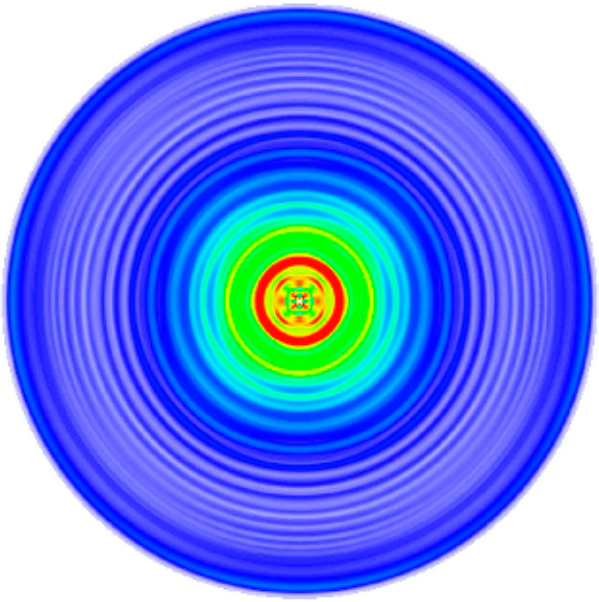

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Study of Ca impurity in helium clusters

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Following recent works [1-3], we present path integral Monte Carlo (PIMC) calculations [4] for the structure and energetics of ^4He_N nanodroplets doped with a single calcium atom. Sizes raging from 10 and 40 helium atoms were considered at temperatures of 1, 1.5 and 2 K. Simulations have been carried out using two different He-Ca interactions, Kleinekathöfer [5] and Lovallo [6], which reveal substantial discrepancies regarding the precise location of the Ca impurity with respect to the helium droplet and the total energy of the system. The different nature of the He–Ca and He–He interactions has been found to be crutial to understand the marked differences between the PIMC predictions in its classical and quantum mechanical versions.

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